Coupled Physical Models for Extreme-Scale Computing

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Outline

Motivation

Building Blocks for the Direct Simulation of Complex Flows
  1. Supercomputing: scalable algorithms, efficient software
  2. Solid phase - rigid body dynamics
  3. Fluid phase - Lattice Boltzmann method
  4. Gas phase - free surface tracking, volume of fluids
  5. Electrostatics - finite volume
  6. Fast implicit solvers - multigrid

Multi-physics applications
  - Coupling elementary models
  - Examples

Perspectives
The Two Principles of Science

Three

Theory
mathematical models, differential equations, Newton

Experiments
observation and prototypes, empirical sciences

Computational Science
simulation, optimization, (quantitative) virtual reality

Computational methods open the path to Predictive Science
Building Block I:

Current and Future High Performance Supercomputers
### Two Multi-PetaFlops Supercomputers

#### JUQUEEN
- Blue Gene/Q architecture
- 458,752 PowerPC A2 cores
- 16 cores (1.6 GHz) per node
- 16 GiB RAM per node
- 5D torus interconnect
- 5.8 PFlops Peak
- TOP 500: #8

#### SuperMUC
- Intel Xeon architecture
- 147,456 cores
- 16 cores (2.7 GHz) per node
- 32 GiB RAM per node
- Pruned tree interconnect
- 3.2 PFlops Peak
- TOP 500: #14

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**What is the problem?**
Designing Algorithms!

with four strong jet engines

Would you want to propel a Superjumbo

or with 1,000,000 blow dryer fans?

Moderately Parallel Computing

Massively Parallel MultiCore Systems
Building block II:

Granular Media Simulations

with the physics engine


Why study granular matter?

consists of discrete, solid, macroscopic particles:

- is ubiquitous in nature,
- is ubiquitous in our daily life,
- is the second-most manipulated material in industry,
- exhibits many complex behaviours,
- eludes the description through unified model equations,
- and is insufficiently understood.
Particle Presentation

A single particle is described by

- its state variables (position \(x\), orientation \(\phi\), translational and angular velocity \(v\) and \(\omega\)),
- a parameterization of its shape \(S\) (e.g. geometric primitive, composite object, or mesh)
- and its inertia properties (mass \(m\), principle moments of inertia \(I_{xx}\), \(I_{yy}\) and \(I_{zz}\)).

The Newton-Euler equations of motion for rigid bodies describe the rate of change of the state variables:

\[
\begin{pmatrix}
\dot{x}(t) \\
\dot{\phi}(t)
\end{pmatrix} = \begin{pmatrix}
v(t) \\
Q(\phi(t))\omega(t)
\end{pmatrix}
\]

\[
M(\phi(t)) \begin{pmatrix}
\dot{v}(t) \\
\dot{\omega}(t)
\end{pmatrix} = \begin{pmatrix}
f(s(t), t) \\
\tau(s(t), t) - \omega(t) \times I(\phi(t))\omega(t)
\end{pmatrix}
\]
Contact Representation

A contact is described by
- the contact location \( \hat{x} \),
- the contact normal \( n \),
- and the signed contact distance \( \xi \).

For a pair of particles \((1, 2)\) with convex shapes \( S_1, S_2 \) and associated signed distance functions \( f_1, f_2 \) these can be defined to be

\[
\hat{x} = \arg \min_{f_2(y) \leq 0} f_1(y), \\
n = \nabla f_2(\hat{x}), \\
\xi = f_1(\hat{x}).
\]
Contact Models (1)

Soft contacts
- are extremely stiff with realistic material parameters,
- require temporal resolution of collision micro-dynamics,
- have unique solutions,
- and exhibit non-differentiable but continuous velocities.

⇒ ordinary differential equations with discontinuous right-hand side

Fig.: Bouncing ball with a soft contact model.
Contact Models (2)

Hard contacts
• require impulses,
• exhibit non-differentiable but continuous trajectories,
• contact reactions are defined implicitly in general,
• have non-unique solutions,
• and can be solved numerically by methods from two classes.

⇒ measure differential inclusions

Fig.: Bouncing ball with a soft and a hard contact model.
Time Stepping

- Discretization of the Newton-Euler differential equations:

\[
\begin{align*}
(x' (\lambda)) &= (x) + \delta t \left( \begin{array}{c}
v' (\lambda) \\
Q(\varphi) \omega' (\lambda)
\end{array} \right), \\
(\varphi' (\lambda)) &= (\varphi) + \delta t M(\varphi)^{-1} \left( \begin{array}{c}
f(\lambda) \\
\tau(\lambda) - \omega \times I(\varphi) \omega
\end{array} \right).
\end{align*}
\]

- Expression for the relative contact velocity:

\[
\delta v'(\lambda) = v'_1 (\lambda) + \omega'_1 (\lambda) \times (\hat{x} - x_1) - v'_2 (\lambda) - \omega'_2 (\lambda) \times (\hat{x} - x_2)
= A^T A \lambda - A^T b.
\]
Time Stepping

<table>
<thead>
<tr>
<th>Non-penetration conditions</th>
<th>Coulomb friction conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi = 0 \perp \lambda_n \geq 0$</td>
<td>$|\lambda_{to}|_2 \leq \mu \lambda_n$</td>
</tr>
<tr>
<td>$\dot{\xi}^+ \geq 0 \perp \lambda_n \geq 0$</td>
<td>$|\delta v_{to}^+|<em>2 \lambda</em>{to} = -\mu \lambda_n \delta v_{to}^+$</td>
</tr>
<tr>
<td>$\ddot{\xi}^+ \geq 0 \perp \lambda_n \geq 0$</td>
<td>$|\dot{\delta v}<em>{to}^+|<em>2 \lambda</em>{to} = -\mu \lambda_n \dot{\delta v}</em>{to}^+$</td>
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</tr>
<tr>
<td>$\frac{\xi}{\delta t} + \delta v'_n(\lambda) \geq 0 \perp \lambda_n \geq 0$</td>
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</tr>
<tr>
<td>$|\delta v'<em>{to}(\lambda)|<em>2 \lambda</em>{to} = -\mu \lambda_n \delta v'</em>{to}(\lambda)$</td>
<td>$|\delta v_{to}^+|_2 = 0$</td>
</tr>
</tbody>
</table>

Signorini condition  impact law  friction cone condition  frictional reaction opposes slip
Regularizing Multi-Contact Problems
Parallelization via domain partitioning

- Objects **known** on all processes whose subdomains intersect with their shape.
- Center of mass determines **owner**
  - performs integration of state variables
- Advanced parallel data structures for contact detection → must avoid $O(n^2)$ algorithm
- Multiple processes can witness a contact
  - lowest rank responsible for treating contact.
- After position integration
  - new objects created
  - obsolete objects removed
  - ownerships transferred
- Sophisticated protocol for synchronization
  - using a single aggregated message exchange
Parallel Computation

Key features of the parallelization:
- domain partitioning
- distribution of data
- synchronization protocol
- subdomain NBGS
- accumulators and corrections
- aggressive message aggregation
- nearest-neighbor communication
Parallel solution

- Subdomain Non-linear Block Gauss-Seidel (NBGS).
- Exchangeable subsystem solver for $F^{-1}$ relaxes single contacts
- Data dependencies to other processes are updated as in a Jacobi method
- Parallel: two message exchanges per iteration
  - Send velocity corrections from shadow copies to owner.
  - Send velocity corrections to shadow copies

Matrix-free implementation avoids the explicit setup of $F$

Communication of velocity corrections instead of contact reactions avoids exchange of contact data.
Shaker scenario with sharp edged hard objects

864 000 sharp-edged particles with a diameter between 0.25 mm and 2 mm.
Dense granular channel flow with crystallization
Scaling Results

- The solver is algorithmically not optimal for dense systems, hence cannot scale unconditionally, but is highly efficient in many cases of practical importance.
- Strong and weak scaling results for a constant number of iterations performed on SuperMUC and Juqueen.
- Largest ensembles computed
  - $2.8 \times 10^{10}$ non-spherical particles
  - $1.1 \times 10^{10}$ contacts
- Granular gas: scaling results

![Weak-scaling graph on the SuperMUC supercomputer.](image)

![Weak-scaling graph on the Juqueen supercomputer.](image)

![Time-step profile of the granular gas executed with $5 \times 2 \times 2 = 20$ processes on a single node.](image)

![Time-step profile of the granular gas executed with $8 \times 8 \times 5 = 320$ processes on 16 nodes.](image)
waLBerla

Massively Parallel Multiphysics Framework

- Focus on lattice Boltzmann method
- Hybridly parallelized (MPI + OpenMP)
- painstakingly optimized:
  - machine-specific kernels for max performance
- all data structures exa-scalable

Computational Fluid Dynamics with waLBerla

with: F. Schornbaum, C. Godenschwager, E. Fattahi:
Simulation of phantom vocal fold geometry
Summary of Performance on Coronary Geometry

- Weak scaling on JUQUEEN with 458,752 processes
  - over a trillion (10^{12}) fluid lattice cells
    - Cell sizes of 1.27\(\mu\)m (diameter of red blood cells about 7\(\mu\)m)
    - 2.1 \(10^{12}\) cell updates per second
    - 0.41 PFlops

- Strong scaling at cell sizes of 0.1 mm
  - In excess of 6000 time steps per second on 32,768 cores of SuperMUC
    - 2.1 million fluid cells

Single Node Performance

JUQUEEN

SuperMUC

vectorized
optimized
standard
Strong Scaling (Coronary Tree)
TRT, 0.05 mm cell size

SuperMUC
Multi-Physics Simulations for Particulate Flows

Parallel Coupling with waLBerla and PE

with D. Bartuschat and K. Gustavsson (KTH Stockholm)
What can we do with Exa-Scale Computers?

Fluidized Bed:

Even if we want

- to simulate a billion ($10^9$) objects (particles): we can do a billion ($10^9$) operations for each of them in each second

- a trillion ($10^{12}$) finite elements (finite volumes) to resolve the flow between particles: we can do a million ($10^6$) operations for each of them in each second

Fluidized Bed
(movie: thanks to K.E. Wirth, Erlangen)
Fluid-Structure Interaction
direct simulation of Particle Laden Flows (4-way coupling)


Mapping Moving Obstacles into the LBM Fluid Grid

An Example
Mapping Moving Obstacles into the LBM Fluid Grid

An Example (2)

Cell change from fluid to particle
Weak Scaling experiment


Largest simulation on Jugene: 8 Trillion ($10^{12}$)

**Jugene**

**Blue Gene/P**

Densely packed particles

264 331 905 rigid spherical objects
Heterogenous CPU-GPU Simulation

Fluidized Beds:
- Direct numerical simulation
- Fully resolved particles

Fluid-structure-interaction
- 4-way-coupling

Particles: 31250, Domain: 400x400x200, Timesteps: 400 000
Devices: 2 x M2070 + 1 Intel „Westmere“, Runtime: 17.5 h

Conclusions and Perspectives

- Supercomputer power
- Versatile tools
  - Lattice Boltzmann (for flow)
  - Multibody Dynamics (for particles)
  - Multigrid (for electrostatics)
- Limitations when using „mesoscopic“ resolution
  - ensemble size
  - time steps
- Gain insight
  - Multi-Scale
  - Multi-Physics
- Challenges
  - validation
  - software